

Derivation of a numerical method with free second-order derivatives

Young Hee Geum

Department of Applied Mathematics, Dankook University, Cheonan, Korea

Abstract—We have proposed the second-derivative-free numerical method and determined the control parameters to converge cubically. In addition, we have developed the order of convergence and the asymptotic error constant. Applying this iterative scheme to a variety of examples, numerical results have shown a successful asymptotic error constants with cubic convergence.

Keywords—second-derivative-free, order of convergence, asymptotic error constant, iterative method, multiple root, root-finding

1.. INTRODUCTION

MANY researchers[4,5,6,7,8] have been interested in developing the iteration methods and deriving the asymptotic error constant to find the roots of nonlinear equations. The Newton's method is one of the most well-known iteration method and is applied.

Suppose that a function $f : \mathbb{C} \rightarrow \mathbb{C}$ has a multiple zero α with integer multiplicity $m \geq 1$ and is analytic[1,2,3] in a small neighborhood of α . We find an approximated α by a scheme

$$x_{n+1} = g(x_n), \quad n = 0, 1, 2, \dots, \quad (1)$$

where $g : \mathbb{C} \rightarrow \mathbb{C}$ is an iteration function and $x_0 \in \mathbb{C}$ is given. Then we find an approximated α using an iterative method. To solve the equation, we develop the following scheme:

$$g(x) = x - \lambda f(x - \mu h(x)) / f'(x) \quad (2)$$

where

$$h(x) = \begin{cases} f(x)/f'(x), & \text{if } x = \alpha \\ \lim_{x \rightarrow \alpha} f(x)/f'(x), & \text{if } x \neq \alpha. \end{cases} \quad (3)$$

Let $p \in \mathbb{N}$ be given and $g(x)$ satisfy the following relation

$$\begin{cases} \left| \frac{d^p}{dx^p} g(x) \right|_{x=\alpha} = |g^{(p)}(\alpha)| < 1, & \text{if } p = 1. \\ g^{(i)}(\alpha) = 0 \text{ for } 1 \leq i \leq p - 1 \text{ and } g^{(p)}(\alpha) = 0, & \text{if } p \geq 2. \end{cases} \quad (4)$$

Since $g(x)$ is continuous at $x = \alpha$, $g(x)$ is represented by

$$g(x) = \begin{cases} x - \lambda F(x), & \text{if } x = \alpha \\ x - \lambda \lim_{x \rightarrow \alpha} F(x), & \text{if } x \neq \alpha. \end{cases} \quad (5)$$

where $z(x) = x - \mu h(x)$ and $F(x) = \frac{f(x - \mu h(x))}{f'(x)}$.

By Corollary 1 and Corollary 2, we have $[f(z)]_{x=\alpha}^{(k)} = 0$, $0 \leq k \leq m - 1$ and $f(\alpha) = f'(\alpha) = \dots = f^{(m-1)}(\alpha) = 0$, $f^{(m)} \neq 0$. Using L'Hospital's rule repeatedly, we obtain

$$\lim_{x \rightarrow \alpha} F(x) = \frac{[f(z)]_{x=\alpha}^{(m-1)}}{[f'(x)]_{x=\alpha}^{(m-1)}} = 0 \quad (6)$$

The next corollary is useful to calculate $g'(\alpha)$, $g''(\alpha)$ and $g'''(\alpha)$.

Corollary 1: Suppose $f : \mathbb{C} \rightarrow \mathbb{C}$ has a multiple root α with a given integer multiplicity $m \geq 1$ and is analytic in a small neighborhood of α . Then the function $h(x)$ and its derivatives up to order 3 evaluated at α has the following properties with $\theta_j = \frac{f^{(m+j)}(\alpha)}{f^{(m)}(\alpha)}$, $j \in \mathbb{N}$:

(i) $h(\alpha) = 0$

(ii) $h'(\alpha) = \frac{1}{m}$

(iii) $h''(\alpha) = -\frac{2}{m^2(m+1)}\theta_1$

(iv) $h^{(3)}(\alpha) = \frac{6}{m^3(m+1)} \left\{ \theta_1^2 - \frac{2m}{m+2}\theta_2 \right\}$

Corollary 2: Let f stated in Corollary 1 have a multiple root α with a given multiplicity $m \geq 1$. Let $z(x) = x - \mu h(x)$ and $h(x)$ be defined by Eq.(3). Then the following hold:

$$\left. \frac{d^k}{dx^k} f(z) \right|_{x=\alpha} = [f(z)]_{x=\alpha}^{(k)}$$

$$= \begin{cases} 0, & \text{if } 0 \leq k \leq m - 1 \\ f^{(m)}(\alpha) \cdot z'(\alpha)^m, & \text{if } k = m \\ f^{(m+1)}(\alpha) \cdot z'(\alpha)^{m+1} + f^{(m)}(\alpha) \frac{m(m+1)}{2} \cdot z'(\alpha)^{m-1} z''(\alpha), & \text{if } k = m + 1 \\ f^{(m+2)}(\alpha) \cdot z'(\alpha)^{m+2} + f^{(m+1)}(\alpha) \frac{(m+1)(m+2)}{2} \cdot z'(\alpha)^m z''(\alpha) \\ + f^{(m)}(\alpha) \cdot L_{m+2}(\alpha), & \text{if } k = m + 2 \end{cases}$$

where $L_k = \binom{k}{3} t^{k-4} \{ t \cdot (-\mu h''') + \frac{3}{4}(k-3)\mu^2 h''(\alpha)^2 \}$.

2.. CONVERGENCE ANALYSIS

We establish some relationships between λ , m , $g'(\alpha)$, $g''(\alpha)$ and $g'''(\alpha)$, for maximum order of convergence[9,10,11].

We rewrite Eq.(2) into

$$(g - x) \cdot f'(x) = -\lambda f(z). \quad (7)$$

where $f = f(x)$, $f' = f'(x)$ and $z = x - \mu h(x)$ are used for concise and the symbol ' denotes the derivative with respect to x .

Differentiating both sides of Eq(7) with respect to x , we obtain

$$(g' - 1) \cdot f' + (g - x) \cdot f''(x) = -\lambda [f(z)]^{(1)} \quad (8)$$

Since g' is continuous at α , we have

$$g'(x) - 1 = \begin{cases} F_1(x), & \text{if } x \neq \alpha \\ \lim_{x \rightarrow \alpha} F_1(x), & \text{if } x = \alpha, \end{cases} \quad (9)$$

where $F_1(x) = -(g-x)f''(x) - \lambda[f(z)]^{(1)}/f'$.

Using Corollary 2 and $g(\alpha) = \alpha$, we have the following:

$$(g-x)f''(x) \Big|_{x=\alpha}^{(k)} = \begin{cases} 0, & \text{if } 0 \leq k \leq m-2, m \geq 2 \\ (m-1)(g'-1)f^{(m)}(\alpha), & \text{if } k = m-1, \end{cases} \quad (10)$$

$$[f(z)]^{(1)} \Big|_{x=\alpha}^{(k)} = \begin{cases} 0, & \text{if } 0 \leq k \leq m-2, m \geq 2 \\ f^{(m)}(\alpha)(1 - \frac{\mu}{m})^m, & \text{if } k = m-1, \end{cases} \quad (11)$$

Substituting Eq.(10) and Eq.(11) into Eq.(9), we have

$$g'(\alpha) - 1 = -(m-1)(g'(\alpha) - 1) - \lambda(1 - \frac{\mu}{m})^m$$

To obtain $g'(\alpha) = 0$, we get

$$m = \lambda \left(1 - \frac{\mu}{m}\right)^m = \lambda t^m \quad (12)$$

where $t^m = 1 - \frac{\mu}{m}$.

Differentiate both sides of Eq(8) with respect to x , we get

$$g'' + 2(g' - 1) \cdot f'' + (g - x) \cdot f^{(3)} = -\lambda[f(z)]^{(2)} \quad (13)$$

We rewrite

$$g''(x) = \begin{cases} F_2(x), & \text{if } x \neq \alpha \\ \lim_{x \rightarrow \alpha} F_2(x), & \text{if } x = \alpha, \end{cases} \quad (14)$$

where

$$F_2(x) = -2(g' - 1) \cdot f'' - (g - x) \cdot f^{(3)} - \lambda[f(z)]^{(2)}/f'$$

We can get the numerator of $F_2(x)$ by computation similar to that done in $F_1(x)$

$$-2(g' - 1)f'' - (g - x)f^{(3)} - \lambda[f(z)]^{(2)} = \begin{cases} 0, & \text{if } 0 \leq k \leq m-3 \\ f^{(m)}(\alpha)(m - \lambda t^m), & \text{if } k = m-2 \\ f^{(m+1)}(\alpha)[(m+1) - \lambda(t^{m+1} - t^m + t^{m-1})] & \\ -g''f^{(m)}(\alpha)\frac{(m+2)(m-1)}{2}, & \text{if } k = m-1, \end{cases} \quad (15)$$

From Eq.(14) and Eq.(15), we get

$$g'' = \frac{2\theta_1}{m(m+1)} \{(m+1) - \lambda(t^{m+1} - t^m + t^{m-1})\} \quad (16)$$

From Eq.(16), to have $g''(\alpha) = 0$ we get the following relation,

$$m+1 = \lambda(t^{m+1} - t^m + t^{m-1}) \quad (17)$$

Differentiate both sides of Eq.(13) with respect to x to obtain $g^{(3)} \cdot f' + 3g'' \cdot f'' + 3(g' - 1) \cdot f^{(3)} + (g - x) \cdot f^{(4)} = -\lambda[f(z)]^{(3)}$. (18)

We rewrite

$$g^{(3)}(x) = \begin{cases} F_3(x), & \text{if } x \neq \alpha \\ \lim_{x \rightarrow \alpha} F_3(x), & \text{if } x = \alpha, \end{cases} \quad (19)$$

where

$$F_3(x) = -3g''f'' - 3(g' - 1)f^{(3)} - (g - x)f^{(4)} - \lambda[f(z)]^{(3)}/f'\alpha = 1.40449164821534$$

Hence, we have

$$-3g''f'' \Big|_{x=\alpha}^{(k)} - 3(g' - 1)f^{(3)} \Big|_{x=\alpha}^{(k)} - (g - x)f^{(4)} \Big|_{x=\alpha}^{(k)} - \lambda[f(z)]^{(3)} \Big|_{x=\alpha}^{(k)}$$

$$= \begin{cases} 0, & \text{if } 0 \leq k \leq m-4 \\ f^{(m)}(\alpha)(m - \lambda t^m), & \text{if } k = m-3 \\ f^{(m+1)}(\alpha)\{m+1 - \lambda(t^{m+1} - t^m + t^{m-1})\}, & \text{if } k = m-2 \\ -\frac{(m-1)(m^2+4m+6)}{2}g^{(3)}f^{(3)} + f^{(m+2)}(\alpha)(m+2) & \\ -\lambda\{f^{(m+2)}(\alpha)t^{m+2} - f^{(m+1)}(\alpha)\theta_1\frac{m+2}{m}(t^m - t^{m+1}) & \\ -f^{(m)}(\alpha)L_{m+2}(\alpha)\}, & \text{if } k = m-1, \end{cases} \quad (20)$$

Consequently, we have

$$g^{(3)}(\alpha) = \frac{6}{m(m+1)(m+2)}$$

$$\left[\theta_2(m+2) - \lambda\{\theta_2 t^{m+2} + \theta_1^2(t^m - t^{m+1})\frac{m+2}{m} + L_{m+2}(\alpha)\} \right] \quad (21)$$

$$\text{where } L_k = \binom{k}{3} t^{k-4} \{t \cdot (-\mu h''(\alpha)) + \frac{3}{4}(k-3)\mu^2 h''(\alpha)^2\}$$

Theorem 1: Let $f : \mathbb{C} \rightarrow \mathbb{C}$ have a zero α with integer multiplicity $m \geq 1$ and be analytic in a small neighborhood of α . Let θ_1, θ_2 be defined as in Corollary 1. Let t be a root of $\rho(t)$ defined in (20). Let x_0 be an initial guess chosen in a sufficiently small neighborhood of α . Then iteration method (2) with $\mu = m(1-t)$ has order 3 and its asymptotic error constant η as follows:

$$\eta = \frac{1}{6} |g^{(3)}(\alpha)| = \frac{1}{m(m+1)(m+2)} |\phi_1 \theta_1^2 + \phi_2 \theta_2|,$$

where $\phi_1 = -t^{m-2} \lambda q_1(t)$, $\phi_2 = m+2 - \lambda t^{m-2} q_2(t)$, $q_1(t) = -\frac{(m+2)(t-1)^2 \{2(m+1)t - m + 1\}}{2m(m+1)}$ and $q_2(t) = t(t^3 - 2t + 2)$.

3.. NUMERICAL RESULTS

In these experiments, we choose 300 as the minimum number of digits of precision by assigning $\$MinPrecision=250$ in Mathematica to obtain the specified nominal accuracy. We set the error bound ϵ to 0.5×10^{-235} for $|x_n - \alpha| < \epsilon$ and evaluate the n^{th} order derivative of the complicated nonlinear functions using the Mathematica[12] command $D[f, \{x, n\}]$.

As an example for the convergence, we investigate the order of convergence and the asymptotic error constant with a function $f(x) = \{x^{10} - \sqrt{3}x^3 \cos(\pi x/6) + 1/(x^2 + 1)\} (x - 1)$ having a real zero $\alpha = 1.0$ of multiplicity 2. We choose $x_0 = 0.92$ as an initial guess. Table 1 verifies cubic convergence. The computed asymptotic error constants are in successful agreement with theoretical asymptotic error constants η up to 10 significant digits. The computed root is rounded to be accurate up to the 235 significant digits.

Our analysis has been further confirmed through more test functions that are listed below:

$$f_1(x) = \cos x - x, \alpha = 0.739085133215161$$

$$f_2(x) = (\sin^2 x - x^2 + 1)(\cos 2x + 2x^2 - 3),$$

TABLE I
CONVERGENCE FOR

$$f(x) = \left\{ x^{10} - \sqrt{3}x^3 \cos(\pi x/6) + 1/(x^2 + 1) \right\} (x - 1)$$

n	x_n	$ x_n - \alpha $	e_{n+1}/e_n^2	η
0	0.9200000000000000	0.800000		
1	0.991249484161490	0.0121355	1.367268100	3.033
2	0.999794338683744	0.000360502	2.685871931	54251
3	0.99999872081448	3.35582×10^{-7}	3.024323988	
4	0.999999999999950	2.91278×10^{-14}	3.033536758	
5	1.000000000000000	2.19446×10^{-27}	3.033542510	
6	1.000000000000000	1.24557×10^{-52}	3.033542510	
7	1.000000000000000	4.01279×10^{-104}	3.033542510	
8	1.000000000000000	4.16489×10^{-207}	3.033542510	
9	1.000000000000000	$-2.89905 \times 10^{-400}$		

TABLE II
CONVERGENCE FOR VARIOUS TEST FUNCTIONS.

$f(x)$	m	x_0	e_n	ν	η
$f_1(x)$	1	0.490	6.13024×10^{-293}	5	0.04875502284
$f_2(x)$	2	1.290	4.51173×10^{-253}	8	0.7835709502
$f_3(x)$	3	1.080	$0. \times 10^{-249}$	10	5.119146433
$f_4(x)$	4	2.190	1.18904×10^{-261}	8	0.5369302217
$f_5(x)$	5	2.270	2.41280×10^{-398}	9	1.11
$f_6(x)$	6	2.790	2.52653×10^{-359}	9	1.096153846
$f_7(x)$	7	2.590	1.92369×10^{-587}	10	3.591527519
$f_8(x)$	8	1.590	1.90760×10^{-308}	8	0.08249684013

$$\alpha = \sqrt{2} \quad f_3(x) = (\sin(\pi x/2\sqrt{2}) - x^4 + 3)(x^2 - 2)^2,$$

$$f_4(x) = (x^8 - 14x^4 \sin(\pi x/4) - 32)(x^2 - 4x + 4) \log(x - 1), \alpha = 2.000000000000000$$

$$f_5(x) = (3x^7 - 37x^4 + 208) \sin(\pi x/2) \log[x - 1]^3, \alpha = 2.000000000000000$$

$$f_6(x) = (e^{(x^2+7x-30)} - 1)(x - 3) \sin^4 \pi x/3, \alpha = 3.000000000000001$$

$$f_7(x) = (e^{-x} \sin x + \log[1 + (x - \pi)^2])(x - \pi) \sin^3 x (\log[x - \pi + 1])^2, \alpha = \pi$$

$$f_8(x) = (x^2 \sin(\pi x/8) + e^{(x-2)^2} - 1 - 2\sqrt{2})(x - 2)^3 \sin^4(\pi x/2), \alpha = 2.000000000000000$$

Table 2 shows convergence behavior for the above test functions with the multiplicity m , the initial guess x_0 , the least iteration number ν and the asymptotic error constant η . In the future study, we develop extended optimal iteration methods of higher order.

ACKNOWLEDGMENT

Young Hee Geum was supported by the National Research Foundation of Korea funded by the Ministry of Education, Science and Technology (Project No. 2011-0014638).

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